CHE-457/505: Fall 2016 Syllabus

Physical Chemistry for Graduate Students

CHE 457/505

Monday, Wednesday, and Friday

9:00-9:50 AM, Bell Hall 138

Instructor: Prof. Alexey Akimov, NSC 716, 716-645-4140

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Office Hours: Wed. 3 - 4 pm and by appointment. Unannounced visits are discouraged.

Tentative Schedule:

Weeks 1-2: Math intro: derivatives, integrals, differential equations, linear algebra

Weeks 3-4: Phenomenological kinetics, approximate methods (quasi-equilibrium, steady state), enzymatic catalysis, theories of chemical kinetics including charge transfer.

Weeks 5-6: Phenomenological thermodynamics, equation of state, 1-st and 2-nd laws of thermodynamics, thermodynamic potentials, Maxwell equations

Weeks 7-8: Chemical equilibrium, electrochemistry, crystal structure

Exam # 1

Weeks 9-10: Revision of classical mechanics: Hamiltonian and Lagrangian formalisms, equations of motion

Weeks 10-11: Statistical thermodynamics: microstates and Gibbs ensembles, partition function and its relationship to thermodynamic parameters

Weeks 12-13: Fundamentals of quantum mechanics: experimental foundations, mathematical apparatus, Dirac notation, Schrodinger equation. Particle in the box, Harmonic oscillator.

Weeks: 14-15: Hydrogen atom. Perturbation theory and variational method. MO-LCAO. Many-electron wavefunctions and Slater determinants.

Exam #2

Note that the present schedule is only a tentative one. The order of the topics and the timeframes may be changed, as instructor finds appropriate.

Homework and requirements: Homework must be turned in by the end of class on the due date (usually Friday) or before. No late submissions. Exceptions will only be made in the case of documented emergencies. In total, there are 8 homeworks planned. Each homework will bring you the maximal score of 100 points. Homework must be legibly written, cleanly presented, and accurately assembled. Ideally, in the form of the MS Word document (no PDFs). If you plan to submit a handwritten version, ensure with instructor that it is acceptable. Keep in mind, that if your work is acceptable, it doesn't guarantee scoring penalty for its presentation. In your homework, you are expected to show step-by-step derivations and calculations, clear and sufficiently detailed explanations. If you cannot arrive at the final result, show your efforts – only the most meaningful variant that you think might be the closest to the correct solution. Explain. Your efforts may be rewarded, but only if they are meaningful – just showing a bunch of meaningless derivations/calculations won't bring you points. Discussion of the solution among students is encouraged, but copying is prohibited. Plagiarism will not be tolerated.

Due dates are fixed to keep the overall schedule balanced. No changes will be allowed. Please plan your time accordingly.

Grading Policy: A letter grade will be assigned at the end of the course, based on the final percentage score. The cut off percentages used in the previous five years is as follows: 85 = A, 80 = A-, 75 = B+, 70 = B, 65 = B-, 60 = C+, 55 = C, 50 = C-, 45 = D, 40 = F. The instructor reserves the right to modify the grading scheme if this year's class performs very differently from previous classes. The students should read the official UB Incomplete Policy found at: http://undergrad-catalog.buffalo.edu/policies/grading/explanation.shtml#incomplete

Seminars: Practical classes (seminars) will be held after a few lectures on one or several related topics. The main objective of these classes will be to refine your practical problem solving skills and the understanding of the topics. The students' participation will be the main activity of such classes. The participation will contribute toward your final grades. Seminar will typically precede a homework on the discussed topic.

Bonus points: There are 3 ways you can earn bonus points: a) "Magic Crystals". 3 crystals will be awarded after each homework set – to 3 most interesting, creative, clear, perfect (any of those) solutions. The crystals will be applied to final scores to round up your grade to the nearby or next grade letter, depending on the quantity of the crystals won during the semester and your current standing; b) short (5 min) random quizzes in the beginning of some lectures/seminars. You may be asked general questions pertinent to chemical science, history of chemistry, etc. The questions will be given only once, therefore if you are late in the class, you may not be able to answer the questions (still, you can guess). c) “Unexpected ” tests – a 30 min, in-class test with many questions related to the topics pertinent to the present class. The tests may include the topics we have not covered yet.

Course Project:

The course project is expected to be your original research work (not necessarily the one you work on for your thesis). It may be performed under a faculty supervision. The project should demonstrate a certain degree of originality, dedicated work, and your ability to apply concepts of physical chemistry (not only those we can cover in class). The topic of the project can be chosen by a student, instructor, or a guiding faculty (in any case, the selection must be approved by the instructor). Specific guidelines for the course work and its evaluation will be given in the beginning of the class.

The course project draft must be submitted by the end of September. The score will contribute 1/5 of the total project score. The project progress report must be submitted by Nov. 9 and its score will contribute 2/5 of the total project score. The final version of the project paper is due the last day of the class (December 9). The project presentation will take place during the examination week.

Exams: There will be 2 take-home (closed books, no discussion) exams. An oral examination must be passed prior before a student will be allowed to take the written part. The oral part will not be graded, but may delay the start date of your exam (the due date will still be unchanged). Prior to examination, you will be given a list of possible questions. During the oral part you will be expected to explain one or several concepts (and related, if needed) covered in class. On the first meeting you cannot use any external sources. On the following meetings, should they be necessary, you will be allowed to use only your lecture notes (you are allowed to prepare a conspectus in it, based on any external sources).

Weighting scheme:

Just to summarize the overall scheme in computing your grade:

5% - each homework (8 homeworks, total 40%)

5% - participation in class seminars

15% - exam #1

15% - exam #2

5% - course project draft

10% - course project progress report

15% - final version of the course project (10% - written part, 5% - oral presentation)

Extra bonuses: quizzes, "unexpected" tests, and "magic crystals"

Course Website: https://ublearns.buffalo.edu

Academic Integrity: Students should read the official UB Academic Integrity Policy found at: http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml

Students with Special Needs: Please inform the instructor of any special needs and register with the Office of Accessibility Services (ODS) as soon as possible. See http://www.student-affairs.buffalo.edu/ods for details.

Student Resources: A.

University Holidays (No Class): Labor Day (September 5)

Fall Recess (November 23 and 25)

Literature

There is no single textbook for the course. Suggested reading is presented below.

Ask Ben Wagner, a University Librarian, for assistance. I certainly recommend doing this, when preparing your course work.

His contact information: 118 Lockwood Library. Phone: (716) 645-1333. Email: abwagner@buffalo.edu. Info: http://library.buffalo.edu/bwagner

Minimal reading:

1. Brown, LeMay, et al. "Chemistry: The Central Science"

Standard reading:

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1. Thermodynamics, Engel
2. Quantum Chemistry & Spectroscopy, Engel
3. Physical Chemistry: Berry, Rice & Ross
4. Physical Chemistry: Atkins/DePaula
5. Molecular Thermodynamics: R. E. Dickerson
6. Statistical Thermodynamics: D. A. McQuarrie
7. Tom M. Apostol "Calculus": volume 1 - "One-Variable Calculus, with an Introduction to Linear Algebra", volume 2 - "Multi Variable Calculus and Linear Algebra, with Applications to Differential Equations and Probability"

Somewhat advanced reading:

1. Daan Frenkel, Berend Smit "Understanding Molecular Simulations: From Algorithms to Applications";
2. M. P. Allen, D. J. Tildesley "Computer Simulation of Liquids";
3. Frank Jensen "Introduction to Computational Chemistry";
4. L. D. Landau, E. M. Lifshitz "Quantum Mechanics";
5. Shaul Mukamel "Principles of Nonlinear Optical Spectroscopy";
6. I. Prigogine, "Introduction to Thermodynamics of Irreversible Processes";
7. Gene H. Golub, James M. Ortega "Scientific Computing and Differential Equations";
8. Charles Kittel "Introduction to Solid State Physics"